Introduction To Quantum Mechanics

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1 The Wave Function

What we are looking for is the **wave function $\mathbf{\Psi}$**.

Law 1.1 (Schrodinger Equation).

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi.$$

For simplicity, we always rewrite it as:

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_x^2\Psi + V\Psi.$$

Born's statistical interpretation:

$$\int_a^b |\Psi(x,t)|^2 \,\mathrm{d}x = \text{probability of finding the particle between } a \text{ and } b \text{ at time } t.$$

Law 1.2 (Normalization).

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \,\mathrm{d}x = 1.$$

Proposition 1.1. The wave function will always stay NORMALIZED.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \,\mathrm{d}x = 0.$$

Proof. By Schrodinger EQ.,

$$\text{LHS} = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty}.$$

$\square$

Definition 1.1.

$$\langle x\rangle \xlongequal{def} \int_{-\infty}^{\infty} x|\Psi|^2 \,\mathrm{d}x$$

and

$$\langle p\rangle \xlongequal{def} m\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}.$$

Theorem 1.1.
$$\langle x \rangle = \int \Psi^*(x)\Psi \, \mathrm{d}x$$
and
$$\langle p \rangle = \int \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi \, \mathrm{d}x.$$

Remark 1.1 (Operator). We say that the operator x represents position, and the operator $-i\hbar\,\partial/\partial x$ represents momentum. Also,
$$\langle Q(x,p) \rangle = \int_{-\infty}^{\infty} \Psi^* \left[Q(x, -i\hbar \frac{\partial}{\partial x}) \right] \Psi \, \mathrm{d}x.$$

Property 1.1. Operators do **NOT**, in general, commute. For example, $\hat{x}\hat{p} \neq \hat{p}\hat{x}$, i.e.,
$$\exists \text{ a function } f, \text{ s.t. } (\hat{x}\hat{p})f \neq (\hat{p}\hat{x})f.$$

Theorem 1.2 (de Broglie formula). The wave length is related to the momentum of the particle:
$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}.$$

Theorem 1.3 (Heisenberg's uncertainty principle).
$$\sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

2 Time-independent Schrodinger Equation

2.1 Stationary states

We look for solutions that are simple products,
$$\Psi(x,t) = \psi(x)\varphi(t).$$

Theorem 2.1. By the method of separation of variables,
$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi$$
and
$$\varphi(t) = e^{-iEt/\hbar}.$$

The first is called the **time-independent Schrodinger equation**.

Definition 2.1 (Hamiltonian). In classical mechanics, the total energy (kinetic plus potential) is called Hamiltonian:

$$H(x, p) = \frac{p^2}{2m} + V(x).$$

Now we introduce **Hamiltonian operator**:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Thus the time-independent Schrodinger EQ. can be written

$$\hat{H}\psi = E\psi$$

which is **IMPORTANT**.

Remark 2.1. Intriguingly and intuitively,

$$\langle H \rangle = E.$$

Also, if the equation yields an infinite collection of solutions $(\psi_1(x), \psi_2(x), \cdots)$, each with its associated value of the separation constant $(E1, E2, \cdots)$; thus the wave function is:

$$\Psi(x, t) = \sum_{n=1}^{+\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

Particularly,

$$E_n \geq 0 \text{ for all } n$$

2.2 The infinite square well

Suppose

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}.$$

Theorem 2.2. Inside the well, we have

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

and

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

Property 2.1. $\psi_n(x)$ has some interesting and important porperties:

1. They are alternately even and odd, with the respect to the center of the well.
2. They are mutually orthogonal (i.e., $\displaystyle\int \psi_m(x)^* \psi_n(x)\,\mathrm{d}x = \delta_{mn}$) where δ_{mn} is **Kronecker delta**:
$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}.$$
3. They are complete by Dirichlet's theorem.

2.3 The harmonic oscillator

Let
$$V(x) = \frac{1}{2} m\omega^2 x^2.$$

Here I will introduce 2 entirely different approaches to this problem. The first is a diabolically clever algebraic technique and the second is a straitforward "brute force" solution.

2.3.1 Algebraic method

To begin with, let's rewrite the EQ. in a more suggestive form:
$$\frac{1}{2m}\left[\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 + (m\omega x)^2\right]\psi = E\psi.$$

The idea is to factor the term in square brackets:
$$u^2 + v^2 = (u - iv)(u + iv).$$

Definition 2.2 (Ladder operator)**.**
$$\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x).$$

Definition 2.3 (Commutator)**.** The commutator of operators $\hat{A}$ and $\hat{B}$ is
$$\left[\hat{A}, \hat{B}\right] \xlongequal{def} \hat{A}\hat{B} - \hat{B}\hat{A}.$$

Property 2.2.
$$[\hat{a}_-, \hat{a}_+] = 1.$$

Theorem 2.3. If ψ satisfies the Schrodinger's EQ. with energy E, then $\hat{a}_+\psi$ satisfies the Schrodinger's EQ. with energy $E + \hbar\omega$:

$$\hat{H}\psi = E\psi \Longrightarrow \hat{H}(\hat{a}_+\psi) = (E + \hbar\omega)(\hat{a}_+\psi).$$

Similarly,

$$\hat{H}\psi = E\psi \Longrightarrow \hat{H}(\hat{a}_-\psi) = (E - \hbar\omega)(\hat{a}_-\psi).$$

Proof.

$$\hat{H} = a_+a_- + \frac{1}{2}\hbar\omega.$$

□

Here, then, is a wonderful machine for generating new solutions——if we could just find one solution. Thus, we call $\hat{a}_+$ raising operator and $\hat{a}_-$ lowering operator.

But what if I apply the lowering operator **repeatly**? We will reach a state with energy less than zero. By 2.1, there is **NO** guarantee that it will be normalized.

Proposition 2.1. Thus, there occurs a "lowest rung" ψ_0 such that

$$\hat{a}_-\psi_0 = 0.$$

Theorem 2.4.

$$\psi_0(x) = A_0 e^{-m\omega/2\hbar\, x^2}$$

and

$$E_0 = \frac{1}{2}\hbar\omega.$$

Thus we could get

$$\psi_n(x) = A_n(a_+)^n e^{-m\omega/2\hbar\, x^2}, \text{ with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

where A_n are used for normalization.

Theorem 2.5. ψ_n and ψ_{n+1} should satisfy:

$$\begin{cases} a_+\psi_n = i\sqrt{(n+1)\hbar\omega} \\ a_-\psi_n = -i\sqrt{n\hbar\omega}\psi_{n-1} \end{cases}.$$

Proof.

$$\int_{-\infty}^{\infty} |a_+\psi_n|^2 \,\mathrm{d}x = (n+1)\hbar\omega$$

and

$$\int_{-\infty}^{\infty} |a_-\psi_n|^2 \,\mathrm{d}x = n\hbar\omega.$$

$\square$

Ultimately,

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}}.$$

2.3.2 Analytic Method